

RESONANCE SPIN FILTER

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Abstract

During last years the world-community of nano-electronics is engaged in a search of new physical principles, materials and technologies on which the quantum spin-transistor may be manufactured [1]. This anticipated device could become a base of the toolbox of quantum computations and help testing the constructions of various quantum networks.

Basic principle of the spin-transistor was suggested in the paper [1]. The leading idea of the proposal is the use of the spin-orbital interaction [2] for creation of the spin-polarized current in the transistor channel. Actually, to produce a real device based on the above mentioned principle one should:

1. select proper material with maximal spin-orbital interaction causing a considerable spin-orbital splitting,
2. suggest a method of introduction and withdrawal of electrons with certain spin polarization.

An extended analysis of experimental and theoretical ideas leading to the solution of the first problem was suggested in the pioneering paper [3]. According to [4, 5, 6] the maximal spin splitting may appear in semiconductors with Kane dispersion for spectral bands. The magnitude of splitting is bigger for materials with smaller Kane gap, see [7]. Generically, the spin-orbital splitting is two times bigger in the semiconductors with inverse band structure, compared with other semiconductors, see [6, 8].

In the simplest phenomenological Rashba model for the non-symmetric quantum well the corresponding additional linear term with Rashba parameter α is added to the quadratic kinetic term:

$$E^{\pm} = \frac{\hbar^2 k^2}{2m} \pm \alpha k. \quad (1)$$

The Rashba parameter α is defined by the band structure of the material, in particular by the magnitude Δ_R of the gap, by the quasi-momentum, by the electrostatic potential $V(z)$ forming 2D- electron gas and by the shape of the wave-functions of 2d electrons. According to [3, 4, 5] both the theory and the experiment vote in favor of materials Cd Hg Te, where Δ_R circa 40 – 60 meV, and the magnitude of the effective Rashba parameter is about $(0.2 - 0.3)10^{-10}$ eV/m. This is approximately 10 times bigger, that the parameter α in other hetero-structures studied before : $\Delta_R \approx (0.02 : 5)$ meV and $\alpha \approx (10^{-12} - 10^{-11})$ eV m. We guess that such materials as Cd Hg Te are most prospective for the high-temperature Spintronics. Analysis done in [5, 6, 8] shows that large values of spin-orbital splitting are also achieved for InAs and HgTe. All these semi-conductors are representatives of the class of narrow-gap materials with the quasi-relativistic dispersion function and wide spectral bands.

In semiconductors with a nearly parabolic dispersion curve $E \approx \frac{\hbar^2 p^2}{2m^*}$ the magnitude of the expected splitting is at least 2 or 3 orders less than in narrow-gap materials listed

above, hence it is hardly accessible for observations. Nevertheless in actual note we suggest a theoretical analysis of resonance transmission across the quantum well in a material with parabolic dispersion curve and the Rashba Hamiltonian just included additively as in (1), having in mind that it is universal for low temperature and small α . We reveal effects caused by the shape of the oscillatory modes in resonance processes, thus making a step toward the solution of the second of above problems - the problem of introducing and withdrawal of spin-polarized electrons, - actually the problem of registration of the spin-polarization. We calculate transmission coefficients for the Resonance Spin Filter designed in form of a quantum network consisting of a quantum well with three semi-infinite quantum wires (an input wire and two terminals) attached to it. Transmission of electrons across the well from the input quantum wire to terminals is caused by the excitation of the resonance oscillatory mode in the well. The resonance mode is non-symmetric with respect to the spin-inversion and hence the spin-selection can be achieved via special choice of the geometry of the well and contact points of terminals on the boundary of it.

Analysis of the spin-independent resonance transmission was done in [?, 13], where optimization of transport properties was achieved based on distribution of zeroes of the normal derivatives of the resonance mode on the border of the well. An essential difference of the actual problem from the previous one is the fact, that the resonance eigenfunctions in actual problem are *complex* two-component spinors, hence the corresponding one-pole approximation for the Scattering matrix, see (11) below, is presented via 2×2 block's which contain characteristics of the shape of the resonance mode on the border of the well and play the roles of transmission-reflection coefficients for electrons with spin up or down. Nevertheless the optimization of selection can be achieved based on the explicit formula (11).

1 Hamiltonian and the Intermediate Hamiltonian

Consider a network $\Omega = \Omega_0 \cup \omega_1 \cup \dots$ on (x, z) plane combined of a circular quantum well Ω_0 and three straight semi-infinite quantum wires ω_s , $s = 1, 2, 3$ of constant width δ attached to the well Ω_0 such that the orthogonal bottom sections γ_s of the wires ω_s are parts of the piece-wise smooth boundary $\partial\Omega_0$ of the well Ω_0 . We consider scattering of electrons in the network in presence of a strong electric field directed orthogonally to the (x, z) plane. The wave-function Ψ of the electron is presented by spinor (ψ_1, ψ_2) , and the spin-orbital interaction is taken in form of Rashba Hamiltonian [2] : a cross product - of the vector σ of Pauli matrices and the vector p of momentum of electron :

$$H_R = \alpha [\sigma, p], \quad (2)$$

where α is an absolute constant. In presence of a strong electric field $\mathcal{E} = |\mathcal{E}|e_y$ directed orthogonally to the (x, z) plane the corresponding Schrödinger equation on the well is

$$Lu = -\frac{\hbar^2}{2m^*} \Delta u + Vu + \alpha[\sigma_z p_x - \sigma_x p_z]u \quad (3)$$

where $\alpha[\sigma_z p_x - \sigma_x p_z] = (H_R)_y$ is the y -component of the cross product $\alpha[\sigma, p]$, and the linear potential $V := |\mathcal{E}|y$ on the well is defined by the macroscopic electric field \mathcal{E} . The

above Rashba Hamiltonian is non-self-adjoint in the space $L_2(\Omega)$ but the whole Schrödinger operator (3), is a self-adjoint operator in $L_2(\Omega)$ on the domain of sufficiently smooth functions with appropriate conditions imposed on their boundary values, see (5,6). On the wires the potential is constant $V = V_\infty$, but we assume that the Schrödinger equation on the wires $\omega_s = \{0 < \eta_s < \delta, 0 < \xi_s < \infty\}$ contains an anisotropic tensor of effective mass:

$$lu = -\frac{\hbar^2}{2m^\parallel} \frac{d^2 u}{d\xi^2} - \frac{\hbar^2}{2m^\perp} \frac{d^2 u}{d\eta^2} + V_\infty u, \quad (4)$$

and the width of wires is constant and equal to δ . We neglect the spin-orbital interaction in the wires. On the sum $\Gamma = \sum_{s=1}^3 \gamma_s$ of bottom sections of the wires, separating the wires from the well, we impose proper matching boundary conditions on the boundary of the well:

$$\frac{\hbar^2}{2m^*} \frac{\partial u}{\partial n} - \frac{i\alpha}{2} [\sigma, n] u \Big|_{\partial\Omega_0 \setminus \Gamma} = 0, \quad (5)$$

$$\frac{\hbar^2}{2m^*} \frac{\partial u}{\partial n} - \frac{\hbar^2}{2m^\parallel} \frac{\partial u_s}{\partial n} - \frac{i\alpha}{2} [\sigma, n] u \Big|_{\gamma_s} = 0, \quad (6)$$

They define a self-adjoint operator \mathcal{L} on $L_2(\Omega)$ which plays a role of the Hamiltonian of the electron on the network. Following the pattern of [13] we consider the scattering problem for \mathcal{L} on the network Ω and calculate the transmission coefficients from the input wire ω_1 to the terminals ω_2, ω_3 across the well and estimate the quantum conductance on resonance energy, based on Landauer formula, see [9, 10].

Denote by $e_l = \sqrt{\frac{2}{\sqrt{2m^\perp}\delta}} \sin \frac{\pi l \eta}{\sqrt{2m^\perp}\delta}$, $l = 1, 2, 3, \dots$, $0 < \eta < \delta$ the eigenfunctions of the cross-sections of the wires and assume that the Fermi level in the wires lies in the middle of the first spectral band in the wires $E_F = V_\infty + \frac{5}{2} \frac{\hbar^2}{2m^\perp} \frac{\pi^2}{\delta^2}$. Denote by P_+ the orthogonal projection onto the linear hull of the entrance vectors $\bigvee_s e_{1,s} = E_+$ of the open first channel, and by P_- the complementary projection in $L_2(\Gamma)$: $I = P_+ + P_-$. We define the *Intermediate Hamiltonian* $\hat{\mathcal{L}}$ by the same Schrödinger differential expressions (3, 4) but replacing the matching conditions (6) by the “chopping-off” boundary conditions in open channels:

$$P_+ u_s \Big|_{\gamma_s} = 0, \quad s = 1, 2, 3. \quad (7)$$

and the matching conditions in closed channels :

$$P_- [u_0 - u_s] \Big|_{\gamma_s} = 0, \quad \frac{\hbar^2}{2m^*} P_- \frac{\partial u_0}{\partial n} - \frac{\hbar^2}{2m^\parallel} P_- \frac{\partial u_s}{\partial n} - \frac{i\alpha}{2} [\sigma, n] P_- u_0 \Big|_{\gamma_s} = 0. \quad (8)$$

Note that the boundary term $\frac{i\alpha}{2} [\sigma, n]$ arising from the Rashba Hamiltonian commutes with projection onto the entrance vectors of the channels. The operator $\hat{\mathcal{L}}$ on the network defined by the above differential expressions (3, 4) with the boundary conditions (8,7) and the Meixner conditions at the inner angles of the domain is self-adjoint. The operator $\hat{\mathcal{L}}$ is split as an orthogonal sum $\hat{\mathcal{L}} = \mathbf{1}_1 \oplus L_R$ of the operator $\mathbf{1}_1$ on the open channel in the wires and the operator L_R acting in the orthogonal complement of the open channels. This operator plays a role of an intermediate operator. We will derive an explicit formula for the scattering

matrix in terms of spectral data of L_R , see (9). The spectrum of the part \mathbf{l}_1 of $\hat{\mathcal{L}}_R$ in the open channels is just a semi-axis $V_\infty + \frac{\pi^2 \hbar^2}{2m^\perp \delta^2} < \lambda < \infty$. The absolutely-continuous spectrum of the part L_R of the operator $L_R = \hat{\mathcal{L}} \ominus \mathbf{l}_1$ on the orthogonal complement of the open channels consists of a countable family of branches $\cup_{l=2}^\infty \left[\frac{l^2 \hbar^2 \pi^2}{2\mu^\perp \delta^2} + V_\infty, \infty \right)$.

2 Scattering matrix

Denote by G_R the Green function of the operator L_R . The solution \mathbf{u} of the Dirichlet problem for the former equation with the data $\{u_1, u_2, u_3\} := u_\gamma \in E_+$ on Γ can be presented as

$$u(x) = - \int_\Gamma \left(\frac{\hbar^2}{2\mu^*} \frac{\partial G_R(x, s)}{\partial n_s} - i\alpha[\sigma, n_s] G_R(x, s) \right) u_\gamma(s) d\Gamma := \mathcal{P}u_\gamma.$$

We match u with the Scattering Ansatz $\mathbf{u} = e^{-ip\xi}\nu + e^{ip\xi}S\nu, \nu \in E_+, p = \frac{\sqrt{2\mu^\parallel}}{\hbar} \sqrt{\lambda - V_\infty - \frac{\pi^2}{2\mu^\perp \delta^2}}$ in the first channel :

$$\frac{\hbar^2}{2m^*} P_+ \frac{\partial u}{\partial n} - \frac{i\alpha}{2} [\sigma, n] P_+ u \Big|_{\gamma_s} = \frac{\hbar^2}{2m^\perp} P_+ \frac{\partial u_s}{\partial n}.$$

Taking into account the continuity $[u - u_s] \Big|_{\gamma_s} = 0$ and denoting by \mathcal{D}_R the boundary differential operation $\mathcal{D}_x^R u = \left(\frac{\hbar^2}{2\mu^*} \frac{\partial u}{\partial n} - i\alpha[\sigma, n]u \right)$ and by $\Lambda_R(\eta, \eta')$ the generalized kernel of the corresponding Dirichlet-to-Neumann map (DN-map) Λ_R , see [?], of the operator L_R on Γ : $\Lambda_R(\eta, \eta') = -\mathcal{D}_x^R \mathcal{D}_{x'}^R G_R(x, x')$, with $x|_\Gamma = \eta, x'|_\Gamma = \eta'$, we calculate the DN map $P_1 \Lambda_R P_1 := \Lambda_R^1$ framed by the orthogonal projections onto the entrance vectors $e_{1,s}$ of the first channel : $P_1 = \sum_{s=1}^3 e_{1,s} \langle e_{1,s} |$. This gives the following formula for the scattering matrix :

$$S = - \frac{\Lambda_R^1 + ipI}{\Lambda_R^1 - ipI}. \quad (9)$$

The transport properties of the filter for given temperature T are defined via averaging of the corresponding transmission coefficients S_{s1} over Fermi distribution on the essential spectral interval, $\Delta_T = \{E_F - \kappa T < \lambda < E_F + \kappa T\}$, see for instance [11]. We may obtain a reasonably good approximation for the Scattering matrix, substituting for $\Lambda_R(x, y)$ the corresponding spectral sum over all eigenvalues λ_m of the operator \hat{L}_R on the essential spectral interval, if the interval does not overlap with the continuous spectrum of L_R :

$$\Lambda_R^1(\eta, \eta') \approx - \sum_{\Delta_T} \frac{P_1 \mathcal{D}_x^R \varphi_m(\eta) \langle P_1 \mathcal{D}_{x'}^R \varphi_m(\eta') |}{\lambda_m - \lambda}, \quad \eta, \eta' \in \Gamma. \quad (10)$$

The formulae (9,10) show that the eigenvalues and eigenfunctions of the intermediate operator define the structure of the Scattering Matrix on Δ_T and the transport properties of the spin-filter based on the quantum well. Recovering necessary spectral data of the intermediate operator with the non-standard boundary conditions (7,8) cannot be done with existing commercial software and needs creation of special programs.

Assume that there exist a resonance eigenvalue λ_0 of the operator \hat{L}_R which is equal to the Fermi -level in the wires $\lambda_0 = E_F$. Then on a (small) part of the essential spectral interval defined by the temperature we may substitute the DN-map by the resonance term only.:

$$\Lambda_R^1(\eta, \eta') \approx \Lambda_{essential}^1(\eta, \eta') - \frac{P_+ \mathcal{D}_x^R \varphi_0(\eta) \rangle \langle P_+ \mathcal{D}_{x'}^R \varphi_0(\eta')}{\lambda_0 - \lambda}$$

The residue of the resonance polar term is proportional to the projection onto the one-dimensional subspace spanned by the portion $P_+ \mathcal{D}_x^R \varphi_0(\eta) \Big|_{\gamma_s} = \phi_s$ of the resonance eigenfunction in the entrance subspace of the wire ω_s :

$$\Lambda_R^1(\eta, \eta') \approx \frac{P_1 \mathcal{D}_x^R \varphi_0(\eta) \rangle \langle P_1 \mathcal{D}_{x'}^R \varphi_0(\eta)}{\lambda - \lambda_0} = |\phi|^2 \{P_\phi\}_{s, s'},$$

where $\phi = \oplus \sum_{s=1}^3 \phi_s$, $|\phi|^2 = \sum_{s=1}^3 |\phi_s|^2$. This gives the one-pole approximation for the scattering matrix :

$$S(\lambda) \approx S_{approx}(\lambda) = P_\phi^\perp - \frac{|\phi|^2 + ip(\lambda - \lambda_0)}{|\phi|^2 - ip(\lambda - \lambda_0)} P_\phi, \quad (11)$$

where $P_\phi^\perp = I - P_\phi$. The last formula implies the following expressions for transmission coefficients at the resonance energy $\lambda_0 = E_F$ for low temperature:

$$S_{s1}(\lambda_0) \approx (S_{approx})_{s1}(\lambda_0) = -2 \frac{\phi_s \rangle \langle \phi_1}{|\phi|^2}.$$

Hence the transmission coefficient from the input wire ω_1 to the wire ω_s is represented by the 2×2 matrix constructed as a product of spinors, and the spin-dependent current is calculated based on the relevant version of the Landauer formula, see [10]. In [12, 13] the resonance eigenfunctions are scalar and real. Then the transmission coefficients are defined by the integrals

$$\int_{\gamma_s} e_\eta \frac{\partial \varphi_0}{\partial n}(\eta) d\eta \int_{\gamma_1} e_\eta \frac{\partial \varphi_0}{\partial n}(\eta) d\eta.$$

The selectivity of the devices in [12, 13] is guaranteed by the presence of the zeros of $\frac{\partial \varphi_0}{\partial n}$ in the middle of the bottom section γ_s of the wire s . In our case the intergrands in the corresponding integrals are spinors, and the transmission coefficients are presented by matrices . Using the superscripts \pm for components of spinors with spin $\pm 1/2$ we write down the formulae for transmission coefficients , for instance:

$$-\frac{1}{2} |\phi|^2 S_{s1}^{++}(\lambda_0) = \int_{\gamma_s} e_1(\eta) \left(\mathcal{D}_x^R \varphi_0 \right)^+ \Big|_{\gamma_s}(\eta) d\eta \int_{\gamma_1} e_\eta \left(\mathcal{D}_x^R \varphi_0 \right)^+ \Big|_{\gamma_1}(\eta) d\eta. \quad (12)$$

The magnitude of the transmission coefficients defines the selectivity of the spin-filter. But recovering of details of the parameter regimes of the switch now is more complicated task, that in [12, 13] , since the matrices are complex and the selectivity is not defined by zeros of one real function. Nevertheless, if the geometry of the well and the positions of the contact

zones γ_s are chosen such that, for given electric field, the matrix elements $S_{s1}^{++}(\lambda_0)$, $S_{s1}^{+-}(\lambda_0)$ bigger than $S_{s1}^{-+}(\lambda_0)$, $S_{s1}^{--}(\lambda_0)$, then the electrons with the spin up prevail in the exit wire s , for non-polarized incoming flow in the wire 1. Based on the above formula (11) one can calculate also the position of the resonance in the complex plane (the pole of the Scattering Matrix), which essentially defines the speed of switching. Based on the one-pole approximation one can construct a solvable model, [14] of the spin filter, in form of a quantum graph with the resonance boundary conditions at the node.

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